Cray and AMD
Scientific Libraries

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Libraries for Cray Systems

- Cray LibSci (Mary Beth)
  - XT3 and beyond
  - BlackWidow
  - Current projects
- AMD Core Math Library (Chip)
Cray Contributors

- Mary Beth Hribar: Manager
- Adrian Tate: Sca/LAPACK, Sparse linear algebra
- Bracy Elton: FFTs
- Chao Yang: BLAS, LAPACK, Direct sparse solvers
- John Lewis: Sca/LAPACK, Sparse linear algebra
- Neal Gaarder: libm
- Catherine Knutson: Library builds and integration
Library Goals

• Extend performance and functionality for scalar systems
• Tune vector libraries for BlackWidow architecture
• Collaborate with
  • Researchers to obtain newest algorithms
  • AMD to provide best Opteron libraries
The Cray Roadmap

Purpose-Built HPC Systems

- Cray X1E
- Cray XD1
- Cray XT3

Cray XD1

HPC Optimized Systems

- Cray XT3 Dual-Core
- Hood Dual-Core
- Hood Multi-Core
- BlackWidow
- Eldorado

BlackWidow 2007
Eldorado 2007
Cray XT3 2006
Cray X1E 2006
Baker 2009

Phase I: Rainier
Multiple Processor Types with Integrated User Environment

Phase II: Cascade
Fully Integrated System

This Presentation May Contain Some Preliminary Information, Subject To Change
Cray XT3 Libraries

- Cray XT LibSci
  - ScaLAPACK
  - SuperLU
  - Cray FFTs *
- AMD Core Math Library (ACML)
  - BLAS
  - LAPACK
  - ACML FFTs
  - Random number generators
- Goto BLAS
- FFTW 3.1.1

Available in software release 1.5

* Subset of Cray FFTs that map to ACML FFTs
FFTs on Cray XT3

- FFTs in ACML
  - Provide “plans”
  - Contain OpenMP version
- Add FFTW 3.1.1 in 1.5
- Add Cray FFT interfaces to ACML FFTs in 1.5
- Pre-built plans for FFTW 3.1.1 by end of 2006
- Additional FFT optimizations in 2007
FFT on Cray XT3

- Have license to distribute 3.x and 2.1.5 versions
- FFTW 3.1.1
  - Initial release in 1.5
  - Pre-built plans ("Wisdom") available end of 2006
- FFTW 2.1.5
  - Initial release at end of 2006
  - Included only for MPI FFTW
  - Tuned by demand
- Further optimizations of FFTW 3.x in 2007
Cray XT3 Sparse Support

• Provide tuned sparse BLAS routines for sparse iterative solvers (end of 2006)
  • PETSc
  • Trilinos
  • User-defined

• Direct sparse solvers
  • SuperLU
  • Pardiso in ACML in 2007
Libraries for Cray Systems

- Cray LibSci
  - XT3 and beyond
  - BlackWidow
  - Current projects
- AMD Core Math Library
BlackWidow LibSci

- Extension of X1/X1E LibSci
  - Additional OpenMP support
  - Sparse BLAS
- Further optimizations
  - One-sided communication
  - BlackWidow memory model
X1/X1E LibSci

Single CPU
BLAS
LAPACK
Cray FFTs
Cray Direct Sparse Solver

SM Parallel (OpenMP)
Level 3 BLAS

DM Parallel
BLACS
PBLAS
ScaLAPACK
Cray DMP FFTs

Provide four libraries to support streaming and data size options

MSP/32-bit
default

SSP/32-bit
-hssp

MSP/64 bit
-sdefault64 (-lsci64)

SSP/64-bit
-hssp -sdefault64
BlackWidow Node

- 4 way SMP
- 2 L1 caches and L2 cache on each processor
- Shared L3 cache
- Faster processing speeds
- Lower memory latency
BW LibSci

Single CPU
BLAS
LAPACK
Cray FFTs
Cray Direct Sparse Solver
Sparse BLAS

SM Parallel (OpenMP)
Level 3 BLAS
Cray FFTs
Cray Direct Sparse Solver
LAPACK (subset)

DM Parallel
BLACS
PBLAS
ScaLAPACK
Cray DMP FFTs

Provide two libraries to support data size options

32-bit
default

64-bit
-sdefault64 (-lsci64)

New features: Sparse BLAS, OpenMP FFTs/Sparse Solver/LAPACK
FFTs

- Cache Tuned
- Added OpenMP capability
- DM FFTs are hybrid
  - Tuned with one-sided communication across nodes
    - CAF and/or SHMEM
  - OpenMP within a node
Sca/LAPACK

- OpenMP versions of LAPACK routines:
  - LU
  - Symmetric Tridiagonalization
  - Cholesky
  - QR
- Collaboration with LBNL to vectorize new eigensolver
- Co-array Fortran PBLAS
Sparse Computation Support

- Sparse BLAS routines to support iterative solvers in
  - PETSc
  - Trilinos
  - User-defined
- OpenMP direct sparse solvers
Libraries for Cray Systems

- Cray LibSci
  - XT3 and beyond
  - BlackWidow
  - Current projects
- AMD Core Math Library
Projects across all Cray systems

- Eigensolver assessment
- ScaLAPACK optimization
- Sparse BLAS strategy
Eigensolver Support

- Comparison of Sca/LAPACK eigensolvers
  - Divide and Conquer
  - Bisection
  - MRRR ("Holy Grail")
  - QR
- Provide Beta release of MRRR for XT3 late 2006
- Work done by Adrian Tate
  - Talk: Thursday at 9:25 am
XT3 Matrix 3 10% of spectrum
ScaLAPACK Optimizations

• Exploit fast one-sided communication in
  • BlackWidow
  • Baker

• Introduce more flexible block sizes
  • De-couple two types of blocking
    • Linear algebra block size
    • Distribution block size
  • User can tune two block sizes separately
Sparse BLAS Routines

• Sparse BLAS (single processor) to support iterative solvers:
  • PETSc
  • Trilinos
  • User-defined

• Investigating Epetra in Trilinos
  • Provides parallel sparse BLAS using
    • Single processor sparse BLAS
    • MPI

• Able to tune communication
• Possible interface to PETSc
  • One common parallel sparse BLAS implementation
  • Improve communication performance of PETSc solvers
Library Goals

- Extend performance and functionality for XT3
  - FFTW, Cray FFTs, Goto BLAS
  - Tuned sparse BLAS for better solver performance
- Tune vector libraries for BlackWidow architecture
  - More OpenMP support in LibSci
  - CAF PBLAS
  - Tuned sparse BLAS for better solver performance
- Collaborate with
  - Researchers to obtain newest algorithms
    - MRRR eigensolver
  - AMD to provide best Opteron libraries
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